

WE CLAIM:

1. A method of predicting at least one toxic effect of a test agent comprising:
 - (a) providing nucleic acid hybridization data for a plurality of genes from at least one cell or tissue sample exposed to the test agent;
 - (b) converting the hybridization data from at least one gene to a gene expression measure;
 - (c) generating a gene regulation score from the gene expression measure for said at least one gene;
 - (d) generating a sample prediction score for the agent; and
 - (e) comparing the sample prediction score to a toxicity reference prediction score, thereby predicting at least one toxic effect of the test agent.
2. A method of claim 1, wherein at least one cell or tissue sample is exposed to a test agent vehicle.
3. A method of claim 2, wherein the converting of step (b) comprises normalizing the hybridization data for background hybridization and for test agent vehicle induced expression.
4. A method of claim 2, wherein the gene expression measure is a gene fold-change value.
5. A method of claim 4, wherein the fold-change value is calculated by a log scale linear additive model.
6. A method of claim 5, wherein the log scale linear additive model is a robust multi-array average (RMA).
7. A method of claim 1, wherein the nucleic acid hybridization data has been screened by a quality control process that measures outlier data.

8. A method of claim 1, wherein step (c) comprises dimensional reduction using Partial Least Squares (PLS).
9. A method of claim 1, wherein the sample prediction score is generated with a weighted index score for each gene.
10. A method of 1, wherein the sample prediction score for the agent is generated from the gene regulation score for said at least one gene.
11. A method of claim 10, wherein the sample prediction score for the agent is generated from the gene regulation score for at least about 10 genes.
12. A method of claim 10, wherein the sample prediction score for the agent is generated from the gene regulation score for at least about 50 genes.
13. A method of claim 10, wherein the sample prediction score for the agent is generated from the gene regulation score for at least about 100 genes.
14. A method of claim 1, wherein the toxicity reference prediction score is generated by a method comprising:
 - (a) providing nucleic acid hybridization data for a plurality of genes from at least one cell or tissue sample exposed to a toxin and at least one cell or tissue sample exposed to the toxin vehicle;
 - (b) converting the hybridization data from at least one gene to fold-change values;
 - (c) generating a gene regulation score from the fold-change value for said at least one gene; and
 - (d) generating a toxicity reference prediction score for the toxin.
15. A method of claim 1, wherein step (a) comprises loading nucleic acid hybridization data to a server via a remote connection.
16. A method of claim 15, wherein the remote connection is over the Internet.

17. A method of claim 1, wherein the toxicity reference prediction score is provided in a database.
18. A method of claim 17, wherein the toxicity reference prediction score is derived from a toxicology model
19. A method of claim 18, wherein the toxicology model is selected from the group consisting of an individual toxin model, a toxin class model, a general toxicology model and a tissue pathology model.
20. A method of claim 1, further comprising:
 - (f) generating a report comprising information related to the toxic effect.
21. A method of claim 20, wherein the report comprises information related to the mechanism of the toxic effect.
22. A method of claim 20, wherein the report comprises information related to the toxins used to prepare the toxicity reference prediction score.
23. A method of 20, wherein the report comprises information related to at least one similarity between the test agent and a toxin.
24. A method of claim 16, wherein the hybridization data is contained in a plain text file.
25. A method of claim 16, wherein the hybridization data is contained in a CEL file.
26. A method of claim 1, wherein the nucleic acid hybridization data is annotated with information selected from the group consisting of customer data, cell or tissue sample data, hybridization technology data and test agent data.

27. A method of claim 15, wherein step (a) further comprises selecting at least one toxicity model to predict said at least one toxic effect.

28. A method of providing a report comprising a prediction of at least one toxic effect of a test agent comprising:

(a) receiving nucleic acid hybridization data for a plurality of genes from at least one cell or tissue sample exposed to the test agent and at least one cell or tissue sample exposed to the test agent vehicle to a server via a remote link;

(b) converting the hybridization data from at least one gene to robust multi-array average (RMA) fold-change values;

(c) generating a gene regulation score from the RMA fold-change value for said at least one gene;

(d) generating a sample prediction score for the agent;

(e) comparing the sample prediction score to a toxicity reference prediction score; and

(f) providing a report comprising information related to said at least one toxic effect.

29. A method of creating a toxicology model comprising:

(a) providing nucleic acid hybridization data for a plurality of genes from at least one cell or tissue sample exposed to a toxin;

(b) converting the hybridization data from at least one gene to a gene expression measure;

(c) generating a gene regulation score from gene expression measure for said at least one gene;

(d) generating a toxicity reference prediction score for the toxin, thereby creating a toxicology model.

30. A method of claim 29, wherein at least one cell or tissue sample is exposed to a test agent vehicle.

31. A method of claim 29, wherein the converting of step (b) comprises normalizing the hybridization data for background hybridization and for test agent vehicle induced expression.
32. A method of claim 29, wherein the gene expression measure is a gene fold-change value.
33. A method of claim 32, wherein the fold-change value is calculated by a log scale linear additive model.
34. A method of claim 33, wherein the log scale linear additive model is a robust multi-array average (RMA).
35. A method of claim 29, wherein the generating of step (c) comprises dimensional reduction using Partial Least Squares (PLS).
36. A method of claim 29, wherein step (d) comprises the generation of a weighted index score for each gene.
37. A method of claim 29, wherein the toxicity reference prediction score for the toxin is generated from the gene regulation score for said at least one gene.
38. A method of claim 37, wherein the toxicity reference prediction score for the agent is generated from the gene regulation score for at least about 10 genes.
39. A method of claim 37, wherein the toxicity reference prediction score for the agent is generated from the gene regulation score for at least about 50 genes.
40. A method of claim 37, wherein the toxicity reference prediction score for the agent is generated from the gene regulation score for at least about 100 genes.

41. A method of claim 29, wherein the toxicology model is selected from the group consisting of an individual toxin model, a toxin class model, a general toxicology model and a tissue pathology model.
42. A method of claim 29, further comprising validating the model.
43. A method of claim 42, wherein the validation comprises using a cross-validation procedure.
44. A method of claim 43, wherein the cross-validation procedure is a 2/3 / 1/3 validation procedure.
45. A computer system comprising:
 (a) a computer readable medium comprising a toxicity model for predicting toxicity of a test agent, wherein the toxicity model is generated by a method of claim 29; and
 (b) software that allows a user to predict at least one toxic effect of a test agent by comparing a sample prediction score to a toxicity reference prediction score in the toxicity model.
46. A computer system of claim 45, wherein the software enables a user to compare quantitative gene expression information obtained from a cell or tissue sample exposed to a test agent to the quantitative gene expression information in the toxicity model to predict whether the test agent is a toxin.
47. A computer system of claim 45, further comprising software that allows a user to transmit from a remote location nucleic acid hybridization data from a cell or tissue sample exposed to a test agent to predict whether the test agent is a toxin.
48. A computer system of claim 45, wherein the nucleic acid hybridization data from the sample may be transmitted via the Internet.

49. A computer system of claim 45, wherein the nucleic acid hybridization data is microarray hybridization data.
50. A computer system of claim 45, wherein the nucleic acid hybridization data is PCR data.
51. A computer system of claim 45, further comprising a data structure comprising at least one toxicity reference prediction score.
52. A computer system of claim 45, wherein the data structure further comprises at least one gene PLS score.
53. A computer system of claim 45, wherein the data structure further comprises at least one gene regulation score.
54. A computer system of claim 45, wherein the data structure further comprises at least one sample prediction score.
55. A computer readable medium comprising a data structure comprising at least one toxicity reference prediction score and software for accessing said data structure.